

Improved predictive modeling of white LEDs with accurate luminescence simulation and practical inputs

TracePro® Opto-Mechanical Design Software's Fluorescence Property Utility

TracePro's Fluorescence Property Utility helps users optimize down converting phosphor formulations and excitation LEDs selection in white LED design. It also facilitates the creation of the fluorescence material property in the TracePro model. The macro tool reads the excitation, absorption and emission luminescence spectra of the luminescent material and the relative spectral power distribution of the excitation LED from the manufacturers' datasheet or physically measured data. While useful for white LED design, this tool can also be used to generate a fluorescence property for any type of energy converting material.

The installation file and white LED model example files for the Fluorescence Property Utility are available for download:

http://www.lambdares.com/technical_support/tracepro/utilities/

LEDs for Solid State Lighting

The use of white LEDs for solid-state lighting to address applications in the automotive, architectural and general illumination markets is just emerging. LEDs promise greater energy efficiency and lower maintenance costs. However, there is a significant amount of design and cost optimization to be done while companies continue to improve semiconductor manufacturing processes and begin to apply more efficient and better color rendering luminescent materials such as phosphor and quantum dot nanomaterials.

In the last decade, accurate and predictive opto-mechanical software modeling has enabled adherence to performance, consistency, cost, and aesthetic criteria without the cost and time associated with iterative hardware prototyping. More sophisticated models that include simulation of optical phenomenon, such as luminescence, promise to yield designs that are more predictive - giving design engineers and materials scientists more control over the design process to quickly reach optimum performance, manufacturability, and cost criteria.

White LED Design Forms

There are generally two types of white LED design forms: (1) luminescent materials including phosphors or quantum dots mounted on an LED and (2) three LEDs of primary colors combined. The Fluorescence Property Utility was developed to facilitate the former. Referencing Figure 1, the earliest and most common commercially available design is a blue LED chip exciting a yellow YAG phosphor. Other designs of this type include red and green phosphors applied to a blue LED, a combination of two or more phosphors spanning blue to red applied to a UV or violet LED, and luminescent quantum dots applied to LEDs.

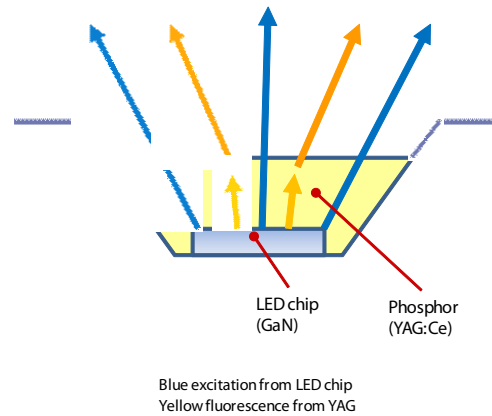


Figure 1. Blue-YAG white LED design form

Performance criteria include luminous flux, relative spectral power distribution, angular intensity distribution and viewing angle. Color criteria includes CIE chromaticity coordinates (x, y), Correlated Color Temperature and Color Rendering Index.

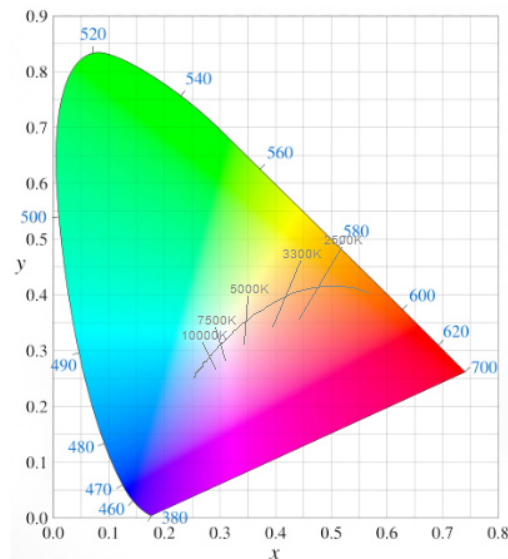


Figure 2. The CIE 1931 x, y chromaticity space showing Planckian locus of blackbody light source chromaticities and iso-temperature lines of constant CCT in degK

Correlated Color Temperature (CCT), used to specify white light, is a comparison of chromaticity coordinates with that of a black body. It is the temperature that corresponds to the blackbody whose chromaticity is represented by the point where the iso-temperature line from the white LED source point intersects the black body curve.

White LEDs may have exactly the same chromaticity coordinates – identical CCT and departure from the Planckian black body locus. However, if they have different spectral distributions of power, they will illuminate a colored object differently and the colored object will have different chromaticity coordinates. The average extent of such differences of chromaticities for a representative variety of colored materials, when calculated for the source under test and a reference source is defined as the Color Rendering Index (CRI). It is a quantitative measure to reproduce colors of various objects in comparison with standardized reference illumination. Exact match of all chromaticities is defined as a CRI of 100.

	CCT (K)
Cool White	4500-10000
Neutral White	3500-4500
Warm White	2670-3500

Figure 3. Representative CCT and CRI for commercially available white LEDs

Predictive Modeling of LED Sources with TracePro

TracePro

TracePro is a comprehensive, versatile software tool for modeling the propagation of light in opto-mechanical systems. Models are created by importing design files from a lens design program or a CAD program or by directly creating the solid geometry in TracePro. Optical and mechanical properties are applied to materials and surfaces. Source rays propagate through the model with portions of the flux of each ray allocated for absorption, specular reflection and transmission, luminescence, and scatter.

From the model, analyze:

- Light distributions in illumination and imaging systems
- Lumens exiting, absorbing, and incident at the component and system levels
- Candela distributions
- Optical efficiency, luminance and radiance metrics
- Luminance effects and lit appearance
- Luminescence effects of phosphors and quantum dots

Modeling Opto-Mechanical Systems in TracePro

TracePro can accommodate a true 3-D model of an LED that provides not only an accurate optical model based on the source modeling described above, but also provides an accurate opto-mechanical model. The opto-mechanical model is created by importing the geometry from mechanical CAD files available from commercial manufacturers or by directly creating the geometry in TracePro based on manufacturers' datasheets.

The user can model the complete packaged LED. Create or import the geometry for the LED cup, LED lens, LED die, etc. and then apply material and surface properties. For higher level system modeling, the user can simply incorporate additional optics and mechanics to the packaged LED source models.

A white LED may be opto-mechanically modeled in software and its adherence to design criteria may be analyzed. In the simple design form in Figure 4, the excitation source, a blue LED is characterized by its relative spectral power distribution and angular intensity distribution. The phosphor material is characterized by relative absorption, excitation and emission spectra, quantum efficiency and its bulk absorption coefficient. Its bulk scatter properties are characterized by wavelength dependent scatter coefficients, anisotropy, and its bulk absorption coefficient.

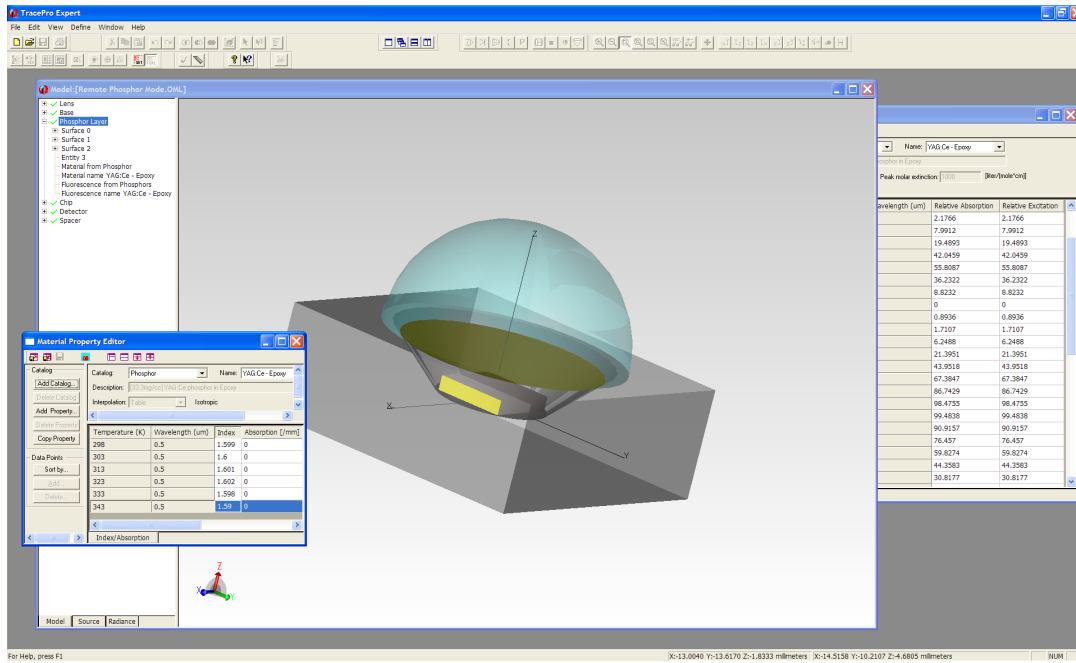


Figure 4. Remote phosphor white LED model in TracePro

Referencing Figure 5, blue LED excitation and yellow luminescence rays are then propagated through the 3-D model with portions of the flux of each ray allocated for absorption, specular reflection and transmission, luminescence, and scatter. From the ray traced model, it is possible to analyze lumens exiting, absorbing, and incident at the component and system levels, candela distributions, optical efficiency, luminance, and radiance metrics.

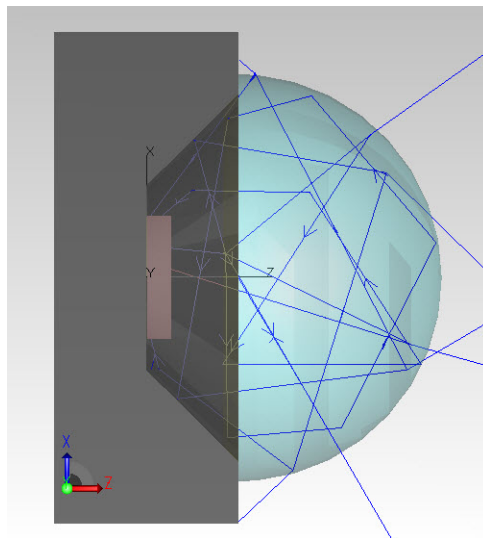


Figure 5. Blue LED excitation and yellow luminescence rays propagating through 3-D solid model in TracePro

TracePro Fluorescence Property Utility

Fluorescence Property Utility

TracePro's Fluorescence Property Utility helps users optimize down converting phosphor formulations and excitation LEDs for white LEDs and then create the fluorescence material property in the TracePro model – quickly and accurately. The macro tool reads the excitation, absorption and emission luminescence spectra of the material and the relative spectral power distribution of the excitation LED from the manufacturers' datasheets. While useful for white LED design, this tool can also be used to generate a fluorescence property for any type of material.

The setup files, example white LED models, and instructions, for installation of the Fluorescence Property Utility may be downloaded at http://www.lambdare.com/technical_support/tracepro/utilities/.

Phosphor Manufacturer's Data

Most often, the optical properties of existing phosphor luminescent material formulations are proprietary. With the goal of discovering an optimum formulation for a particular application, the user, however, can directly import specifications from a phosphor manufacturer's datasheet to TracePro's Fluorescence Property Utility as a starting design point.

Phosphor manufacturers specify relative excitation, absorption and emission spectra for the luminescent material. Referencing Figure 6, below is representative data for a YAG:Ce phosphor.

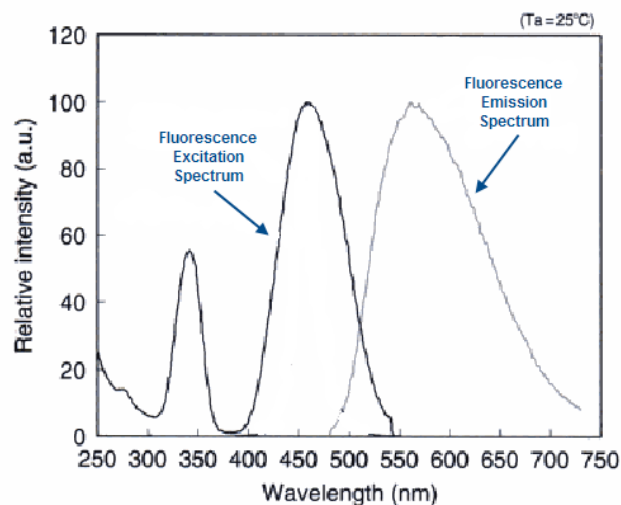


Figure 6. Relative fluorescence excitation and emission spectra for YAG:Ce phosphor

Although not always found in manufacturer's documentation, manufacturers can specify the quantum efficiency, peak molar extinction coefficient (K_{peak}) and molar concentration (C_{molar}) of the supplied phosphor. Sometimes, the manufacturer will specify measured bulk absorption ($u_a(\lambda)$) vs. wavelength as opposed to both peak molar extinction coefficient (K_{peak}) and molar concentration (C_{molar}). From the following relationship, it is possible for the user to calculate inputs to the model depending on the data available.

$$u_a(\lambda) = ab(\lambda) * K_{\text{peak}} * C_{\text{molar}}$$

where $ab(\lambda)$ is the relative absorption spectra.

LED Manufacturer's Data

Similarly, specifications from an LED manufacturer's datasheet or physically measured data can be directly imported to TracePro's Fluorescence Property Editor with the Fluorescence Property Utility.

Relative Spectral Power Distribution

Below are representative Relative Spectral Power Distribution data from Philips Lumileds for Luxeon™ Rebel LEDs and for a theoretical starting design point used as the blue excitation LED in the example that follows.

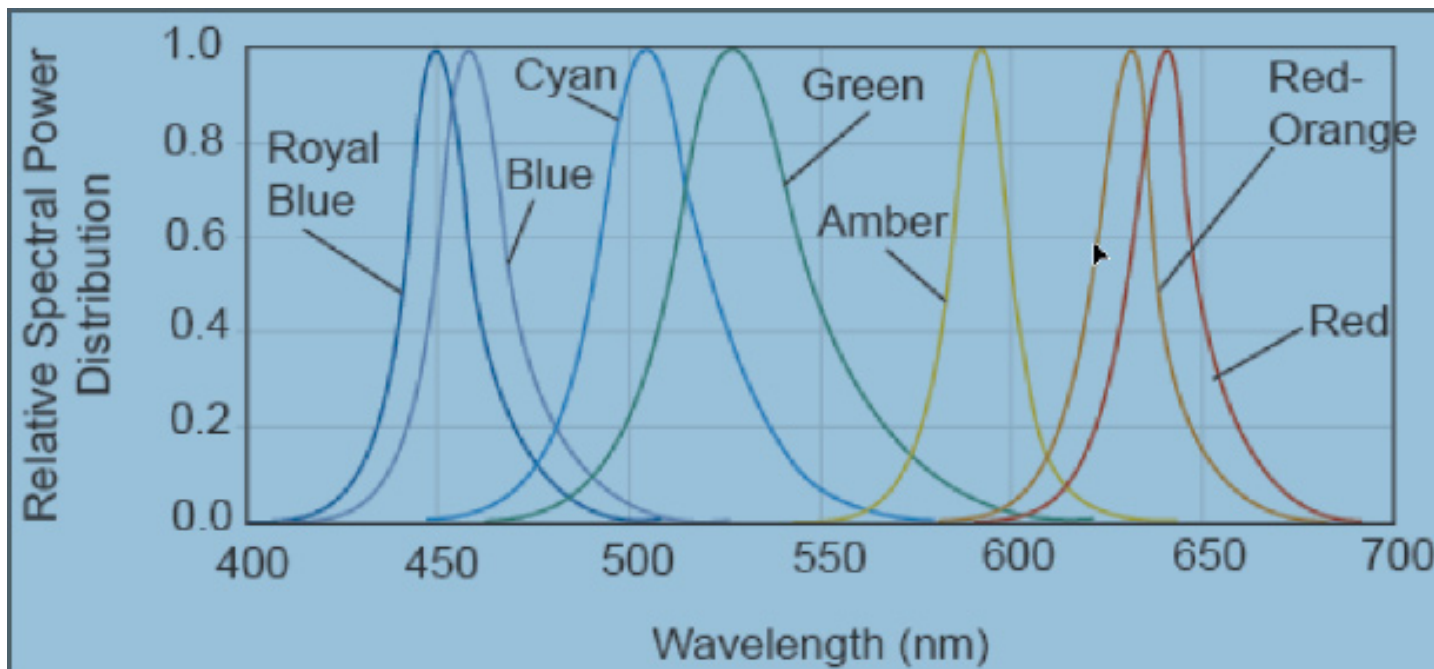


Figure 7. Relative spectral power distribution for LEDs

Optimize Phosphor and Excitation LED Selection with Utility

A step-by-step example using the Fluorescence Property Utility to optimize phosphor formulation and excitation LED selection for white light is given below. The simple design form is a YAG:Ce phosphor excited by a blue LED. The phosphor is defined from its excitation, absorption and emission spectra and its conversion efficiency. The LED excitation source is defined from its relative spectral power distribution.

Phosphor

Import Excitation, Absorption and Emission Spectra

To import the excitation, absorption and emission spectra, first make active the “Fluorescence Property” whiteboard by selecting the “Fluorescence Property” button in the lower right corner of the Utility interface. See Figure 8.

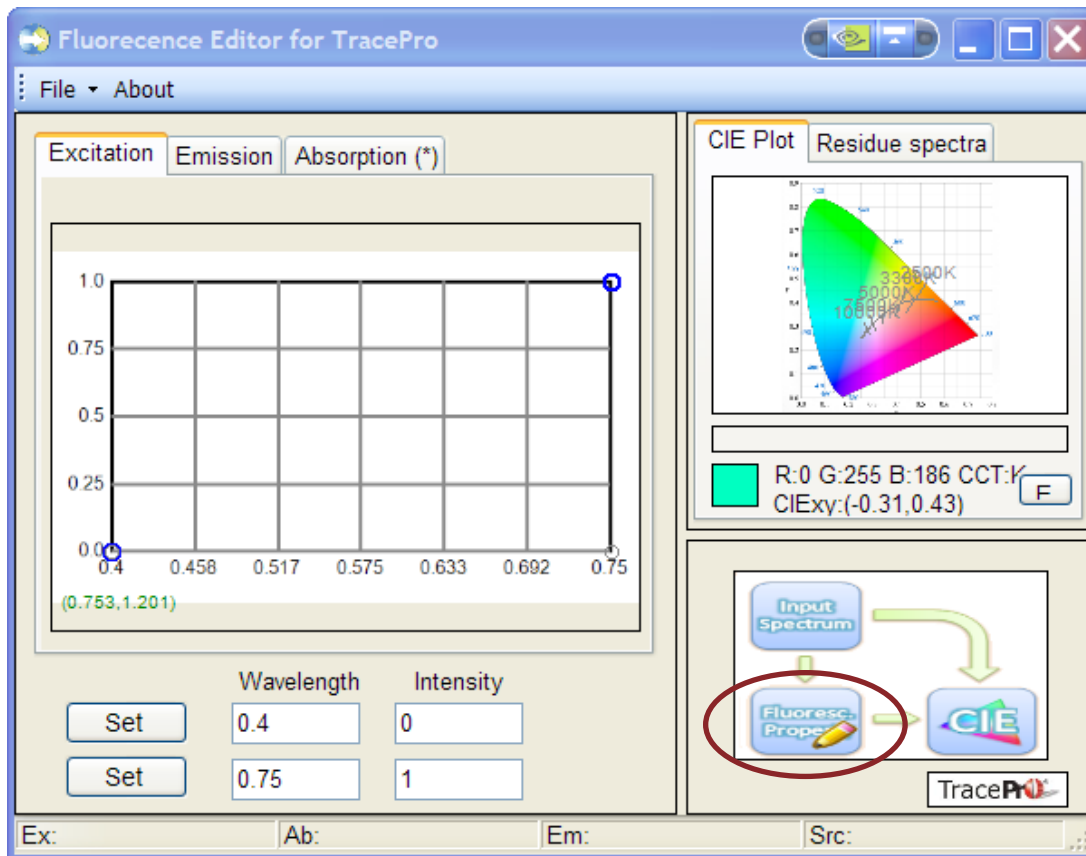


Figure 8. “Fluorescence Properties” whiteboard

Import the phosphor’s excitation spectra by selecting the “Excitation” tab, copying data directly from the datasheet (for this example, copy Figure 6 from this document), and pasting it onto the “Excitation” whiteboard. To paste, right click on the “Excitation” window, and select “Paste” from the menu.

Coordinate System

On the imported curve in the “Excitation” window, identify two reference points. Click “Set Ref1”, go to the graphic window, and click on a reference point. Repeat to select “Set Ref2” below and click on second reference point. It is recommended to set the reference points as far apart as feasible for best accuracy. Specify the “Wavelength” and “Intensity” values for the reference points in the input cells. Notice that wavelengths are specified in the Utility and in TracePro as microns, while phosphor datasheets typically specify wavelength as nanometers (nm).

Referencing Figure 9, the two points identified for the imported YAG:Ce phosphor are at the extremes of wavelength and intensity.

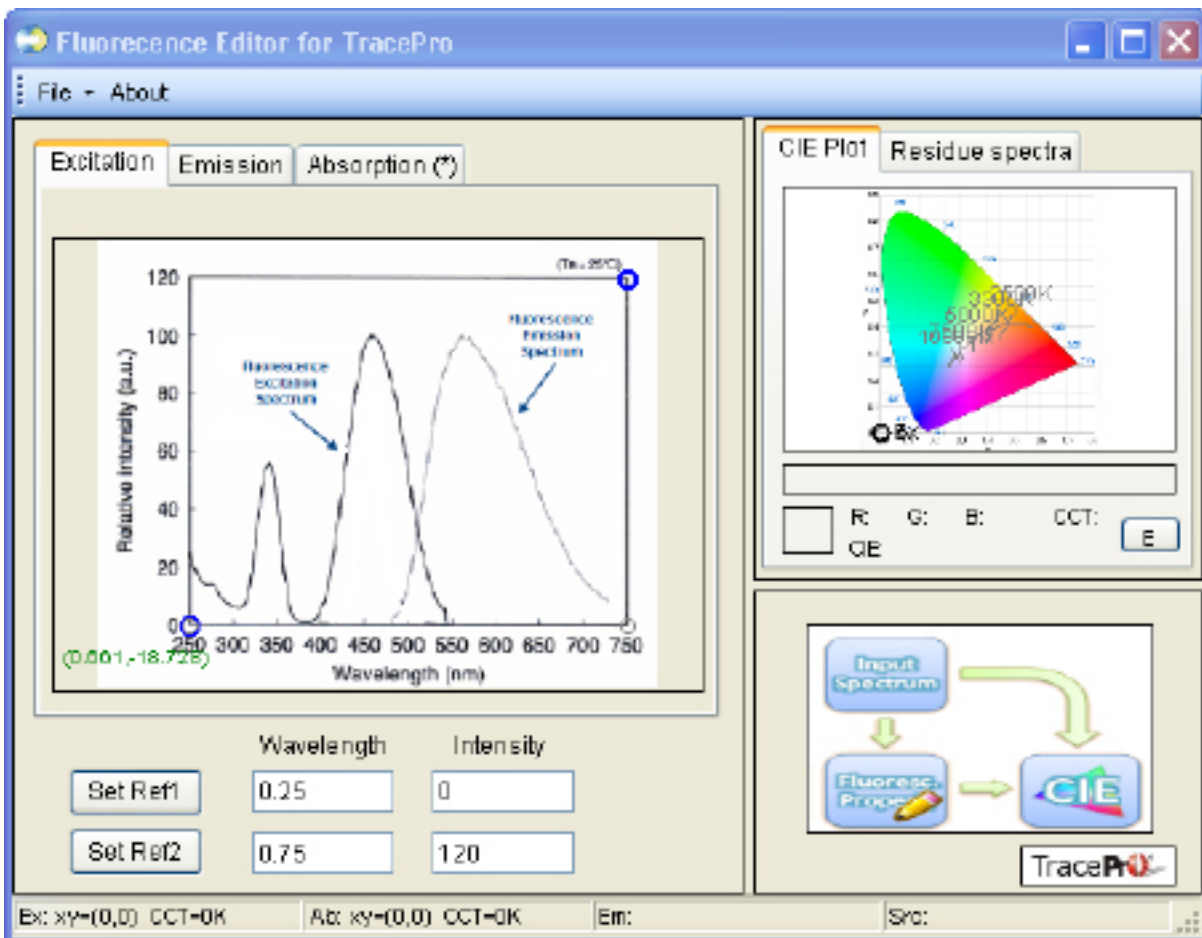


Figure 9. Copy spectra to the “Fluorescence Properties” whiteboard and define coordinate references in “Excitation” window

Set Spectrum Control Points

“Spectrum Control Points” are identified on the imported “Excitation” curve in the “Excitation” window. “Set Data Points” by clicking on the curve in the window. Accuracy improves with number and representative position of data points.

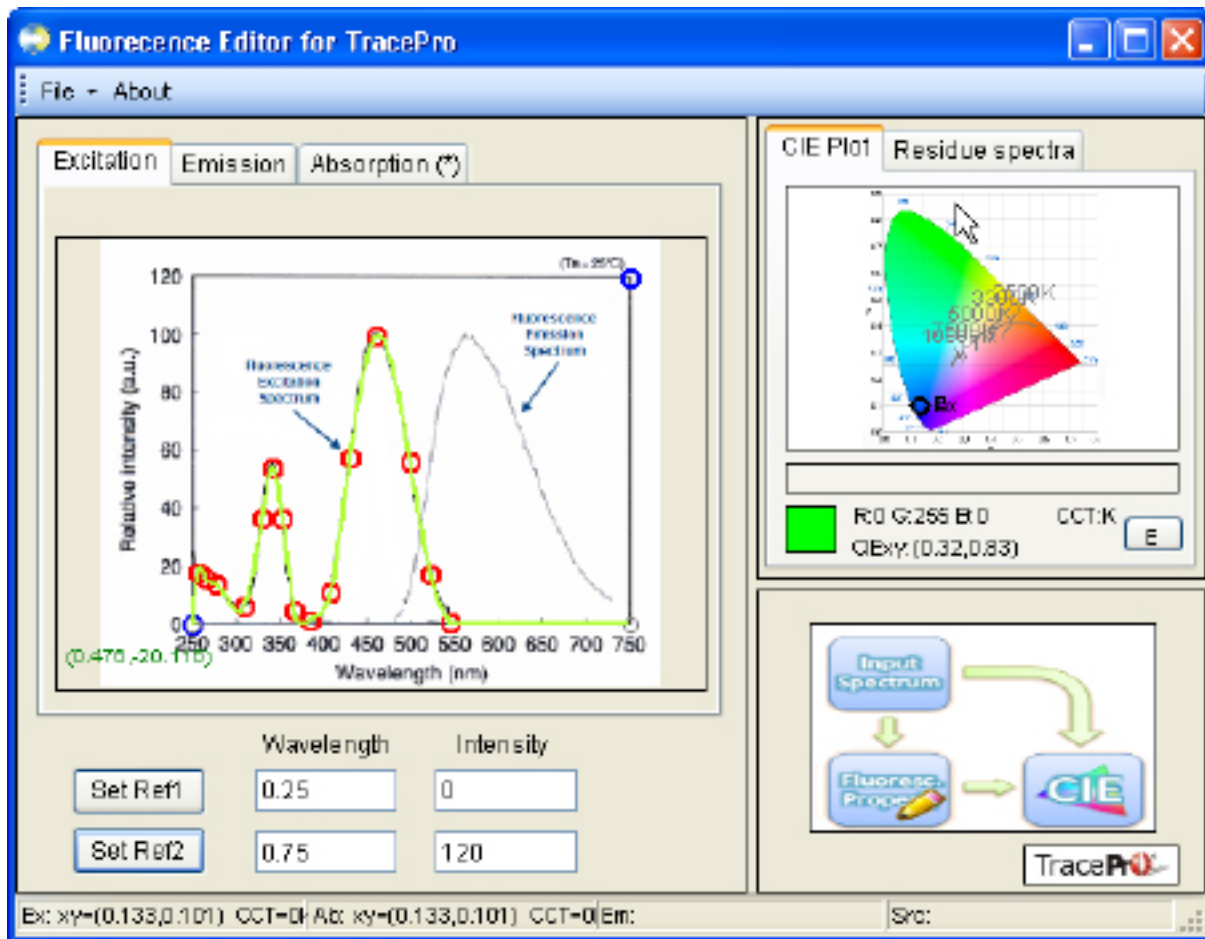


Figure10. Set spectrum control points in “Excitation” window

Additional features for editing and viewing the “Spectrum Control Points” include:

- Move data point by clicking and dragging it
- Delete data point by scrolling over point, right mouse clicking and selecting “Delete”
- Delete all data points by scrolling over any point, right mouse clicking and selecting “Clear All”

Absorption and Emission Spectra

Repeat the above steps to import and define coordinate system and set spectrum control points for the phosphor's emission and absorption spectra.

By default, the excitation curve and its defined control points are automatically copied to the "Absorption" window. This is because most often the excitation and absorption spectra are identical.

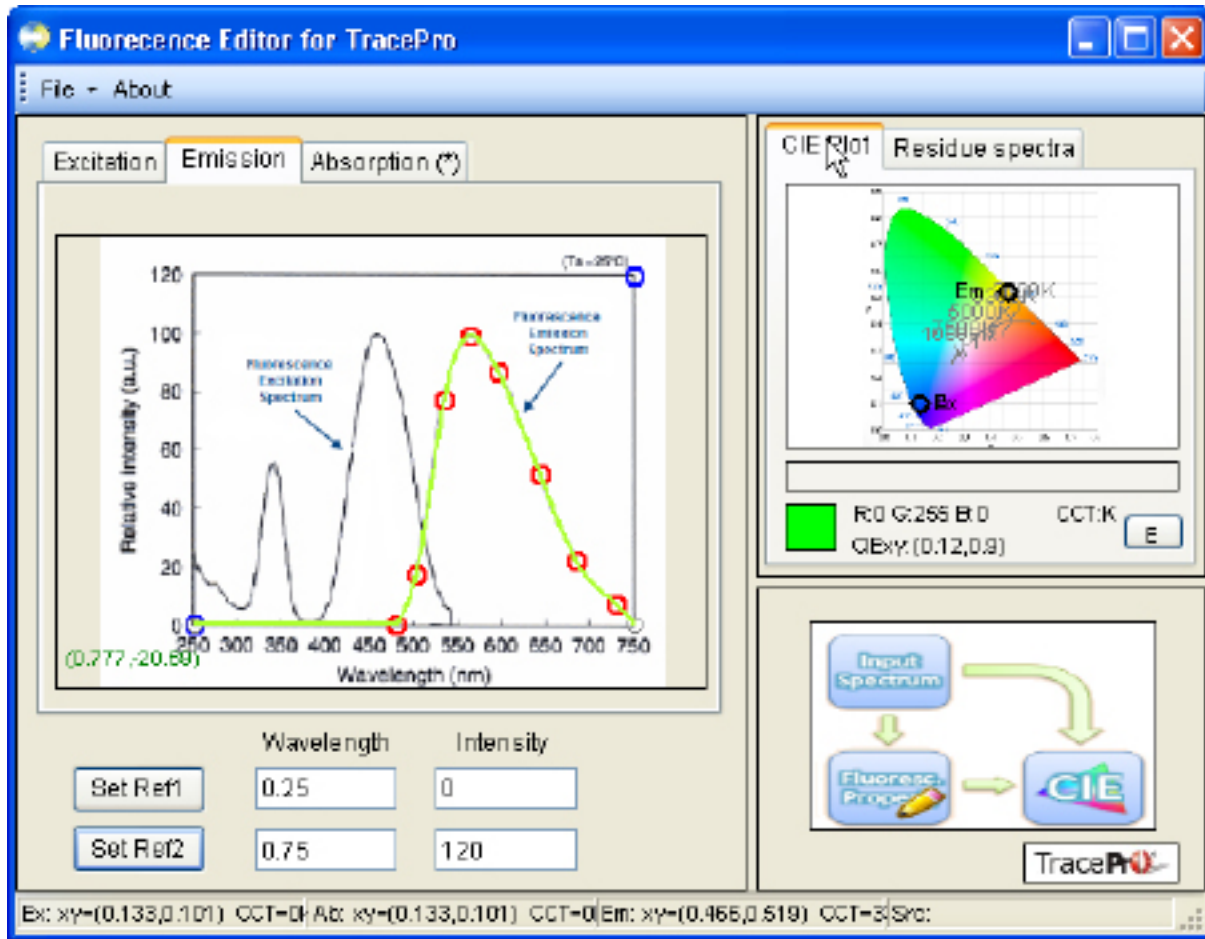


Figure 11. Set spectrum control points in "Emission" window and view YAG:Ce mapped to chromaticity coordinates

CIE Plot

The chromaticity coordinates of the phosphor material's emission, absorption, and excitation energy are determined by its relative emission, absorption and excitation spectra. Referencing Figure 12, the chromaticity coordinates mapped from each spectrum are quantified in the footer bar of the Utility as well as represented on the CIE diagram.

In this example, the emission of the YAG:Ce phosphor yields chromaticity coordinates, (x_{em}, y_{em}) , equal to (0.464, 0.520).

A feature of the "CIE Plot" is that the chromaticity coordinates, RGB value and CCT displayed below dynamically change as the user scrolls over the CIE diagram.

Excitation LED

Import Relative Spectral Power Distribution

To import the “Relative Spectral Power Distribution”, first make active the “Input Spectrum” whiteboard by selecting the “Input Spectrum” button in the lower right corner of the Utility interface. See Figure 12.

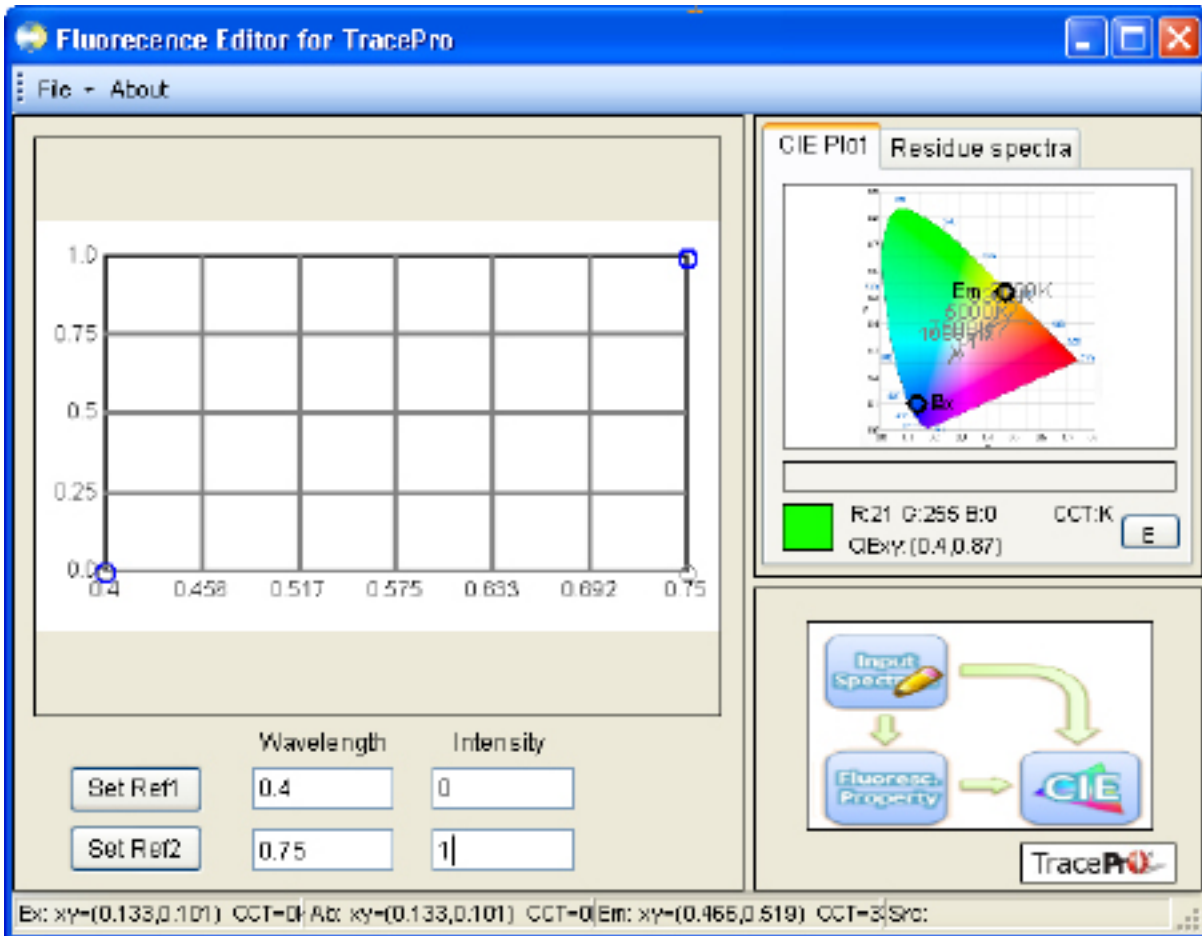


Figure 12. “Input Spectrum” whiteboard

Import "Relative Spectral Power Distribution" by copying data directly from the datasheet (for this example, copy Figure 7 from this document) and pasting it onto the "Input Spectrum" whiteboard. To paste, right click in the "Input Spectrum" window, and select "Paste" from the menu. Referencing Figure 13, Philips Lumileds for Luxeon™ Rebel LED spectra are cut and paste from the manufacturer's data sheet.

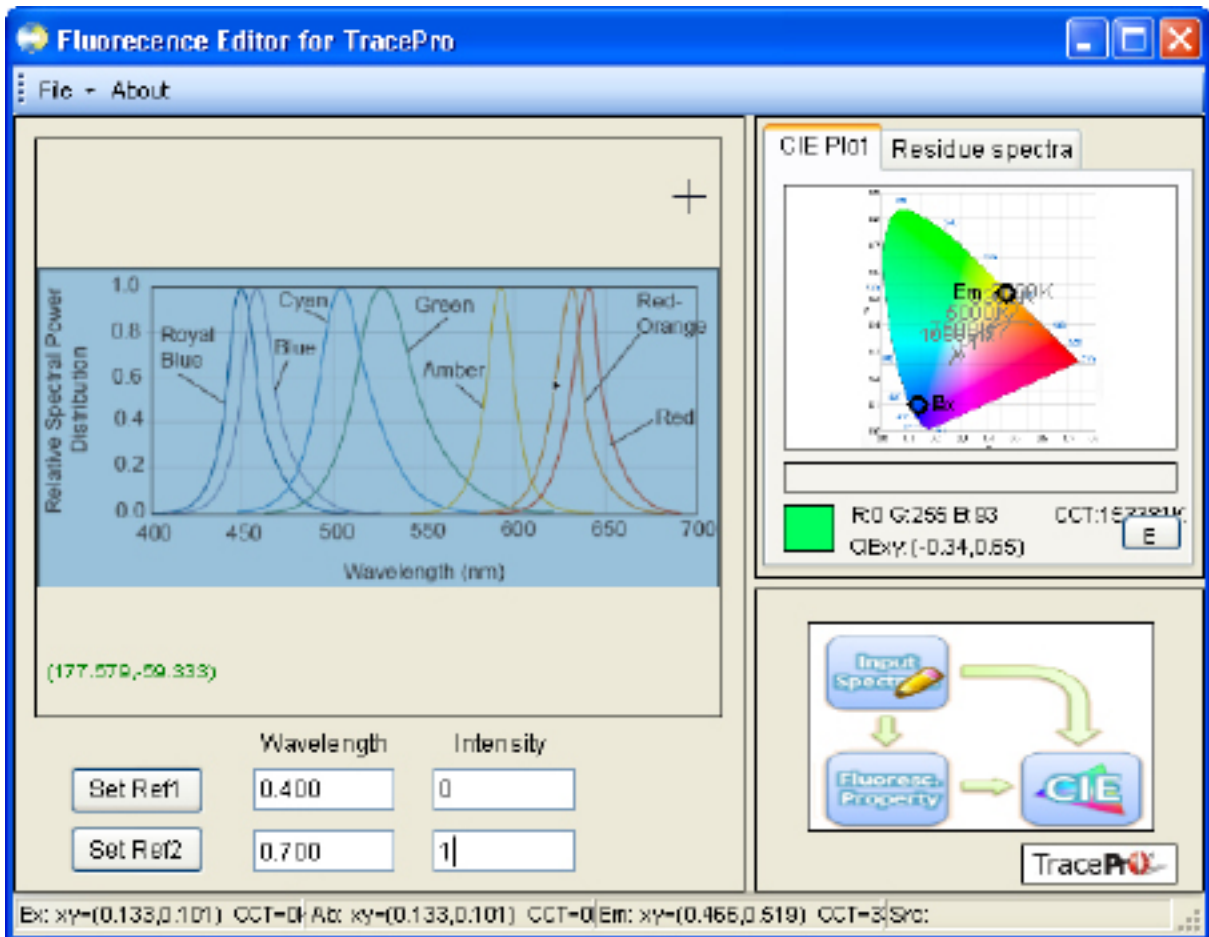


Figure 13. Copy LED spectra distribution spectra to the "Input Spectra" whiteboard

Coordinate System

On the imported curve in the "Input Spectrum" window, identify two reference points. Click "Set", go to the graphic window, and click on a reference curve point. Repeat for second "Set". It is recommended to set the reference points as far apart as feasible for best accuracy. Specify the "Wavelength" and "Intensity" values for the reference points in the input cells. Notice that wavelengths are specified in the Utility and in TracePro as microns, while LED datasheets typically specify wavelength as nanometers (nm).

Referencing Figure 14, the two points identified for the imported LEDs are at the extremes of wavelength and intensity.

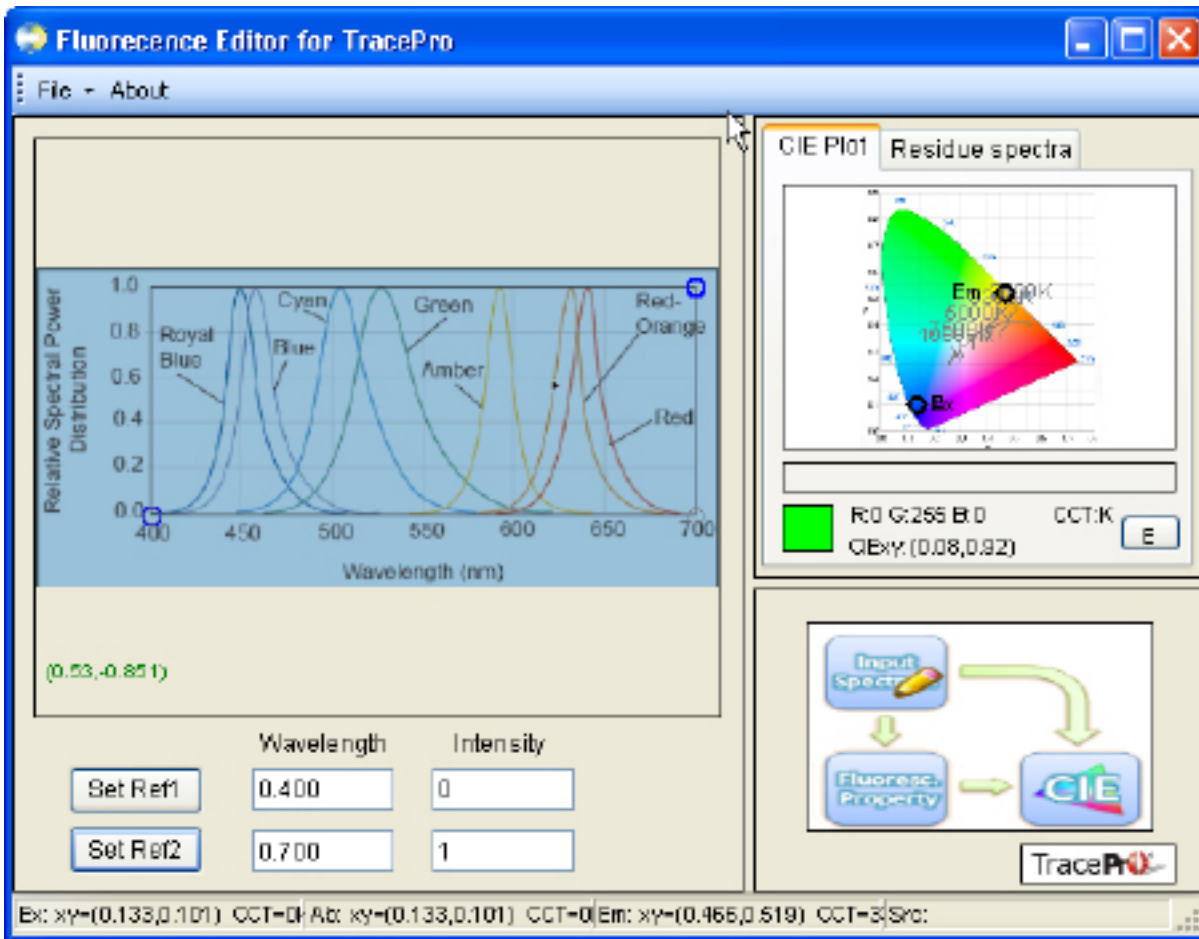


Figure14. Define coordinate references in "Excitation" window

Set Spectrum Control Points

“Spectrum Control Points” may be identified on the imported curve in same way described above when setting spectrum control points for the phosphor’s excitation, absorption and emission spectra. “Set Data Points” by clicking on the curve in the window. Accuracy improves with number and representative position of data points.

Additional features for editing and viewing the “Spectrum Control Points” include:

- Move data point by clicking and dragging it
- Delete data point by scrolling over point, right mouse clicking and selecting “Delete”
- Delete all data points by scrolling over any point, right mouse clicking and selecting “Clear All”

The Utility makes it simple for users to set “Spectrum Control Points” free style with the imported spectrum from manufacturer’s datasheets or measured data as a reference. This is useful for creating design starting points or fine tuning and tolerancing. Referencing Figure 15, “Spectrum Control Points” for a 475nm blue LED are set free style.

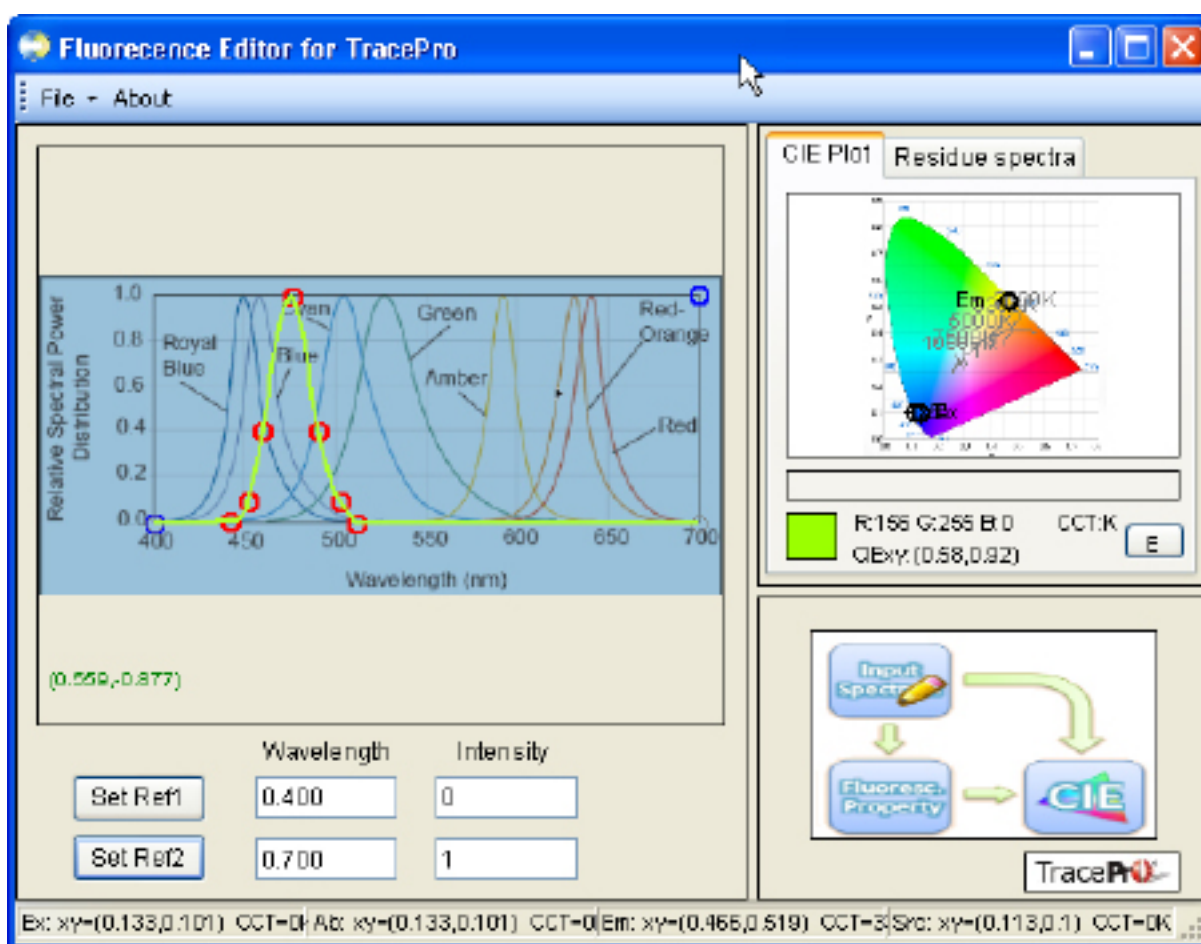


Figure15. Set spectrum control points in “Input Spectrum” window; Relative spectral power distribution of excitation source mapped to chromaticity coordinates

CIE Plot

The chromaticity coordinates of the excitation source are determined by excitation LED’s relative spectral power distribution. This example includes a blue LED as the excitation source where (xsource, ysource) = (0.113, 0.1). Referencing Figure 15, the chromaticity coordinates mapped from each spectrum are quantified in the footer bar of the Utility as well as represented on the CIE diagram.

Color Mix

CIE Plot

White light may result when the blue excitation energy mixes with the yellow luminescence of the phosphor. It is dependent on the chromaticity coordinates of each as well as the conversion efficiency of the phosphor. Click and drag a straight line from Ex (.113, .1) to Em (.466, .519) in the CIE Plot as shown in Figure 16. The line represents the locus of points that result from mixing the blue excitation source energy with the yellow luminescence of the phosphor with different conversion efficiencies.

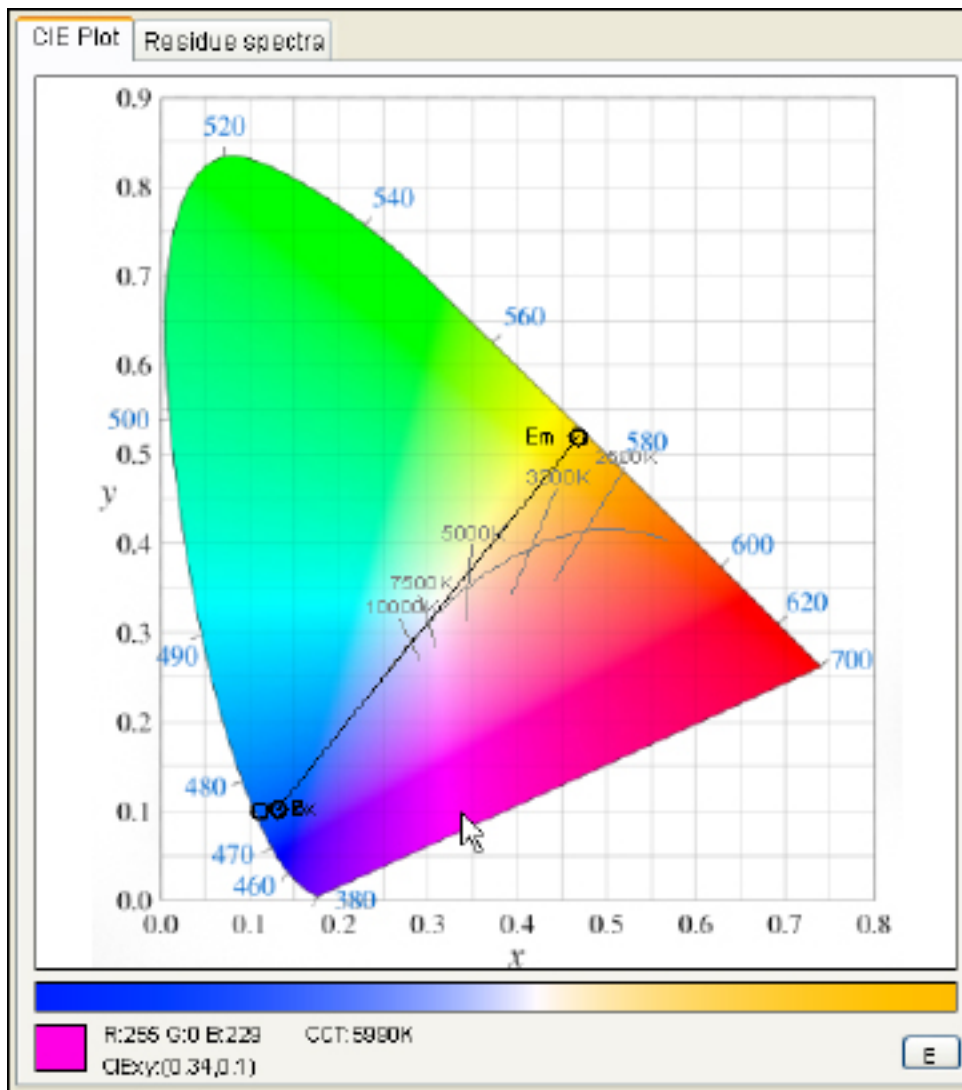


Figure16. Line representing locus of points that result from mixing the blue excitation source energy with the yellow luminescence of the phosphor

Also referencing Figure 16, the color bar below the CIE plot graphically displays the color along the straight line between (xsource, ysource) and (xem, yem). Notice that the chromaticity coordinates, RGB value and CCT displayed below the color bar dynamically change as the user scrolls over the CIE diagram.

Conversion Efficiency

To specify or test the effects of different phosphor conversion efficiencies on the resulting chromaticity coordinates and CCT, select the "Residue Spectra" tab. Referencing Figure 17, move slider at the top of the window to specify the amount of residue excitation energy or 100% minus the conversion efficiency. The plot shows intensity and wavelength of the emission energy and the excitation residue energy relative to that of the original energy of the excitation source. The chromaticity coordinates and CCT of the resulting mix and the residue excitation energy are displayed below the plot.

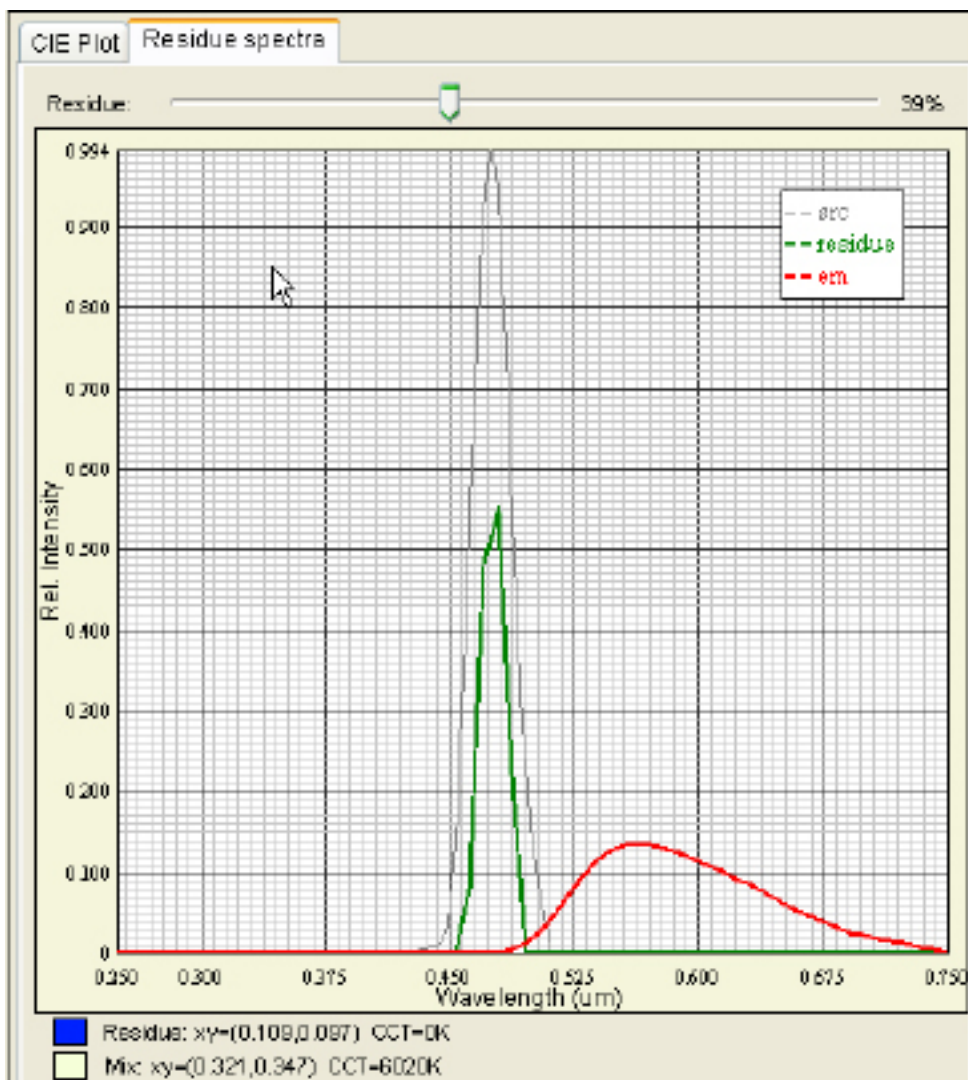


Figure17. White light mix resulting from 39% residual excitation energy

In this example, the CCT of the resulting white light with 61% conversion efficiency or 39% residual excitation energy is shown on the CIE plot at the point, "Mix (39%)". Referencing Figure 3, a conversion efficiency of 61% yields a cool white with CCT of 6136 degK and chromaticity of (0.321, 0.347).

Export Phosphor Properties to TracePro Fluorescence Property

The phosphor formulation and LED excitation source created in the Utility can be directly exported to a Fluorescence Material Property and a Surface Source Property for TracePro. The phosphor data is exported using the same Fluorescence Property Utility used herein. The LED excitation source specified in the Fluorescence Property Utility herein is exported to TracePro with the Surface Source Property Utility. The Surface Source Property Utility and a Technical Note describing its operation and features may be downloaded at

http://www.lambdare.com/technical_support/tracepro/utilities/.

Create TracePro Fluorescence Property

In the top main menu bar of the Utility, select "File" and then "Export TracePro". The "Export Fluorescence Data" dialog box opens. Referencing Figure 18, specify the "Catalog Name" and the "Property Name" where it will be saved in the TracePro Fluorescence Property Database. Enter the "Description" for the new fluorescence property. Then, specify the "Quantum Efficiency", "Peak Molar Extinction" in liter/(mole*cm) and "Temperature" for which this phosphor data and the excitation, absorption and emission spectra defined in the Utility are valid.

Although not always found in manufacturer's documentation, manufacturers can specify the quantum efficiency, peak molar extinction coefficient (K_{peak}) and molar concentration (C_{molar}) of the supplied phosphor. Sometimes, the manufacturer will specify measured bulk absorption ($u_a(\lambda)$) vs. wavelength as opposed to both peak molar extinction coefficient (K_{peak}) and molar concentration (C_{molar}). From the following relationship, it is possible for the user to calculate inputs to the model depending on the data available.

$$u_a(\lambda) = ab(\lambda) * K_{\text{peak}} * C_{\text{molar}}$$

where $ab(\lambda)$ is the relative absorption spectra.

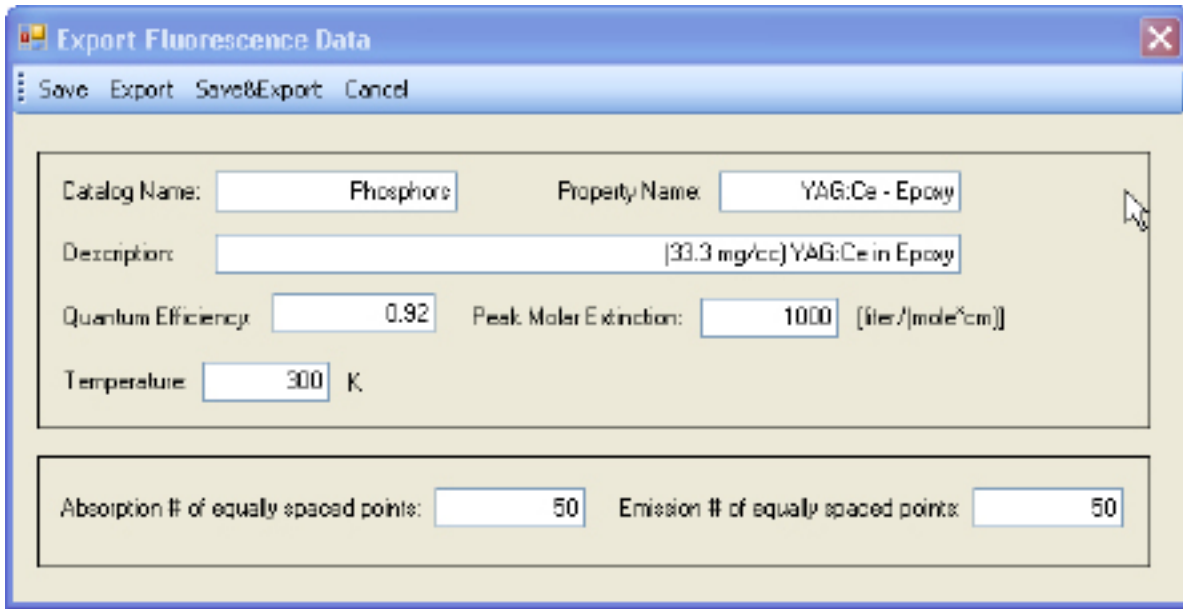


Figure18. "Export Fluorescence Data" dialog box

To export the phosphor data to a TracePro Fluorescence Material Property, open TracePro. Select "Save & Export" in the main menu bar of the "Export Fluorescence Data" dialog box. Referencing Figure 19, save the *.flu file.

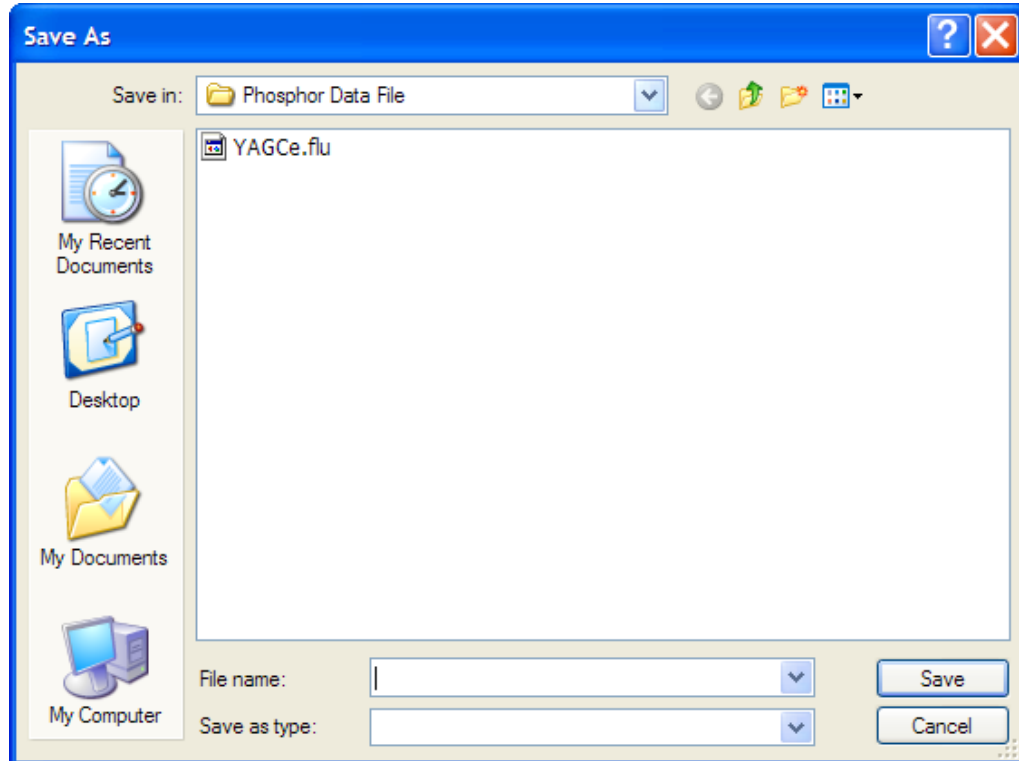


Figure19. "Save As" dialog box for TracePro Fluorescence Material Property

The file is then exported and saved as a Fluorescence Material Property that may be applied to the luminescent component in the TracePro LED model. Referencing Figure 20, the “Fluorescence Property Editor” in TracePro shows the phosphor data created in the Utility and exported to TracePro.

The screenshot shows the 'Fluorescence Property Editor' window. The 'Catalog' section on the left includes buttons for 'Add Catalog...', 'Delete Catalog', 'Add Property...', 'Delete Property', and 'Copy Property'. The 'Data Points' section includes 'Sort by...', 'Add...', and 'Delete...' buttons. The main area displays the following information:

- Catalog: Phosphors
- Name: YAG:Ce-Epoxv
- Description: [33.3 mg/cc] YAG:Ce in Epoxy
- Quantum efficiency: 0.92
- Peak molar extinction: 1000 [liter/(mole²cm)]

Below this information is a table with the following data:

Temperature (K)	Excitation Wavelength (μm)	Relative Absorption	Relative Excitation
300	0.25	0	0
300	0.2602	19.655	19.655
300	0.2704	14.355	14.3334
300	0.2806	13.1266	13.1266
300	0.2908	8.4061	8.3961
300	0.301	4.6514	4.5885
300	0.3112	7.6514	7.5449
300	0.3214	20.5584	20.4826
300	0.3316	40.4432	40.4432
300	0.3418	54.1056	54.1056
300	0.352	38.5119	38.5119
300	0.3622	12.8659	12.6726
300	0.3724	0.2454	0
300	0.3827	0.7951	0.7951
300	0.3929	2.8341	2.8101
300	0.4031	6.9093	6.7889
300	0.4133	20.0039	19.8929

Figure 20. “Fluorescence Property Editor” viewing phosphor data created in and exported from Utility

Predictive White LED Modeling Model

The Fluorescence Property created in the Utility and exported to TracePro is then applied to the luminescent component in a TracePro LED model.

Additional material properties of the phosphor formulation may be incorporated in the model for more accurate simulation. As an example, referencing Figure 21, the designer is able to include temperature dependent data.

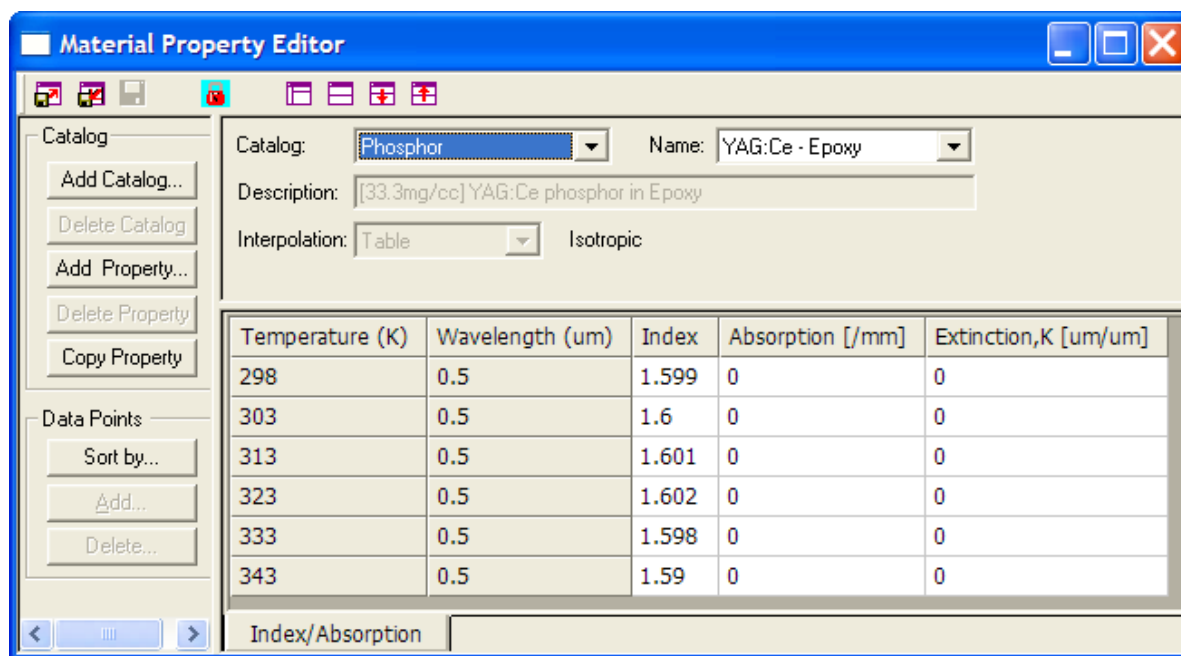


Figure 21. "Material Property Editor" defining refractive index change with temperature

The designer is also able to specify bulk scatter characteristics for the epoxy and phosphor formulation. The ray trace of this model in TracePro then simulates the phosphor formulation's luminescence effects alongside the absorption, reflection, transmission, and scatter effects of the phosphor formulation and other components in the model. The accurate simulation of scatter and luminescence is particularly useful in remote phosphor down conversion designs where backscattered light is extracted from the phosphor layer.

Analysis

From the white LED model, it is possible to analyze luminous flux, relative spectral power distribution, angular intensity distribution and viewing angle at a defined plane in the model. It also possible to analyze color criteria including CIE chromaticity coordinates (x, y) and the Correlated Color Temperature at any defined plane in the model. Referencing Figure 22, TracePro's Candela plot displays the luminous intensity or flux per solid angle.

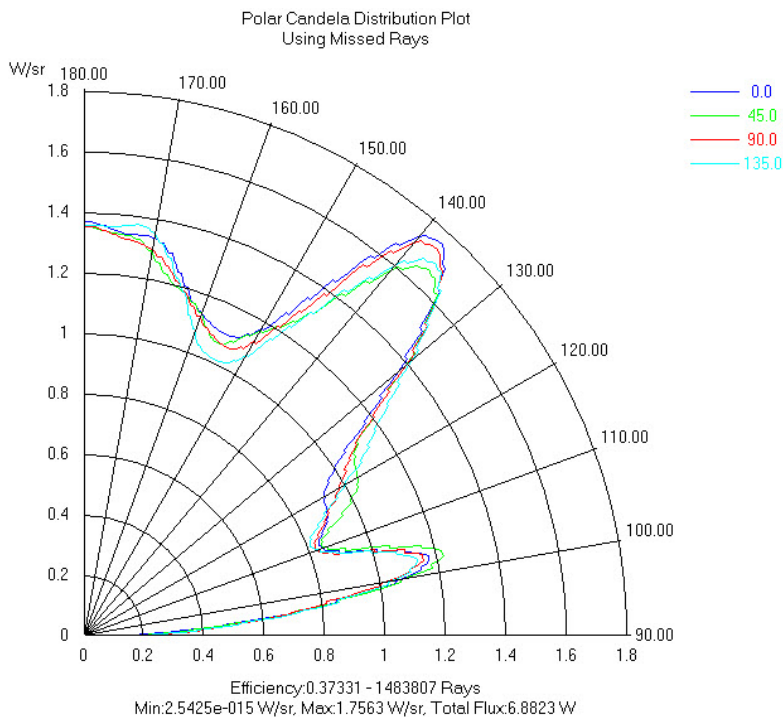


Figure 22. Polar candela distribution plot of Blue YAG white LED

Luminescence Simulation

To simulate luminescence, TracePro traces rays from the LED excitation source to the phosphor. It calculates excitation efficiency, bulk absorption, path length, absorbance and absorption at the phosphor material. The flux in each ray is spectrally weighted as the area ratio of the emission curve. The ratio is the integral under emission curve within the spectral band divided by integral under the entire emission curve. The resulting emission rays are then traced throughout the LED model.

Discrepancies between phosphor down conversion white LED models and experimental data will arise if luminescence simulations do not account accurately for path length related absorbance and absorption, and the phosphor's particle size and particle density. The models described herein account for particle size and density in their excitation and emission spectra and for particle density in molar concentration. Given these inputs, algorithms in TracePro calculate path length dependent absorbance and absorption. The measured bulk scatter property of the phosphor formulation that is integrated into the model also accounts for the phosphor's particle size and density.

Summary

Opto-mechanical Monte Carlo ray trace simulation has been instrumental in the continuous improvements in efficiency, flux, maintenance and cost of white LEDs. How closely the software model predicts the actual device, however, remains dependent on the validity, accuracy and precision of the assumptions and optical property values attributed to each component in the system. For this reason, it is critical that the design software's user interface calls for accurately measured data inputs that are readily available to the designer. Furthermore, in the case of the phosphor down conversion white LED design forms, accuracy of results is also dependent on the fundamental algorithms used to simulate luminescence. More sophisticated simulation algorithms combined with the capability to include accurately measured data inputs give engineers and materials scientists more control over the design process to quickly reach best performance and lowest cost.

For more information, please contact Lambda Research's Application Engineers at sales@lambdaresearch.com.